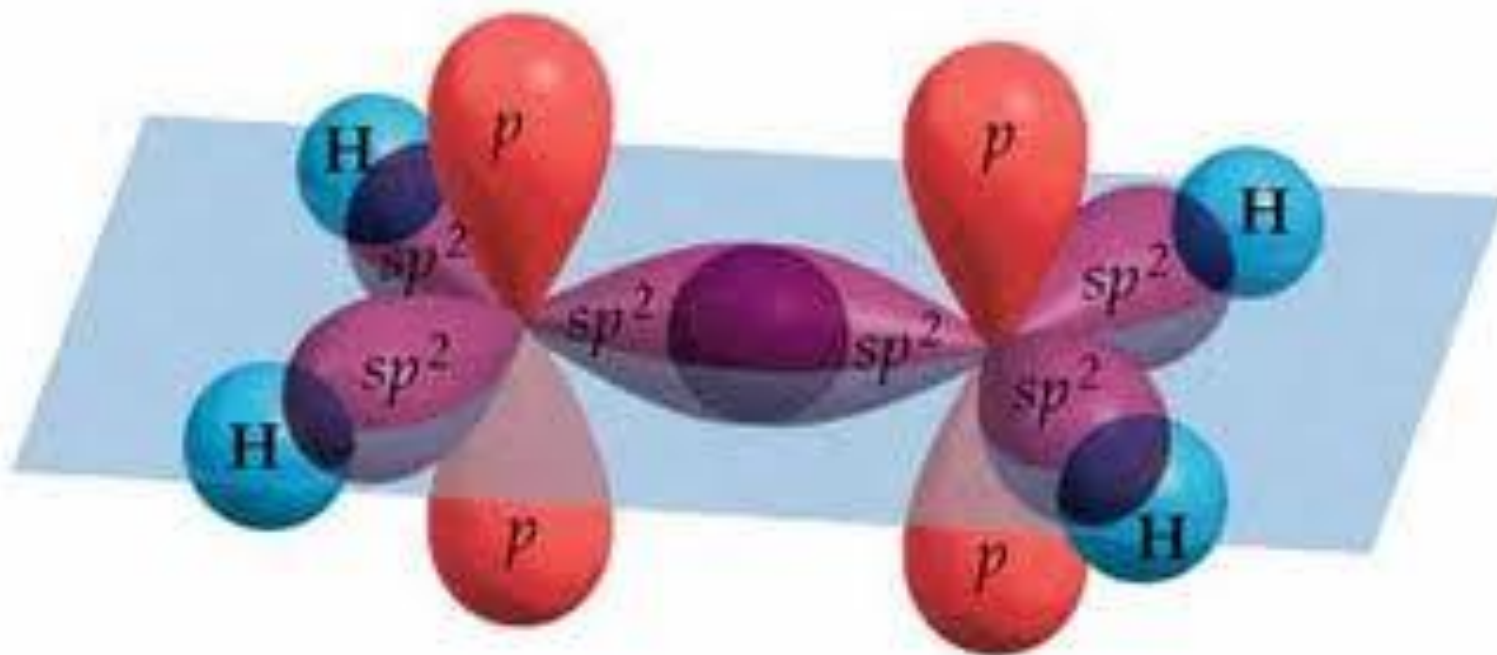
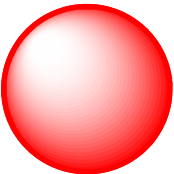


# **Obečná chemie uhlíku a vodíku, orbitaly, hybridizace, vazby, typy reakcí, kinetika a termodynamika**

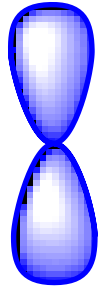
# Teorie orbitalů a vazeb



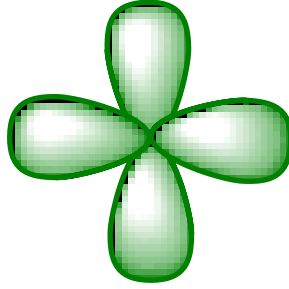
# Atomové orbitaly



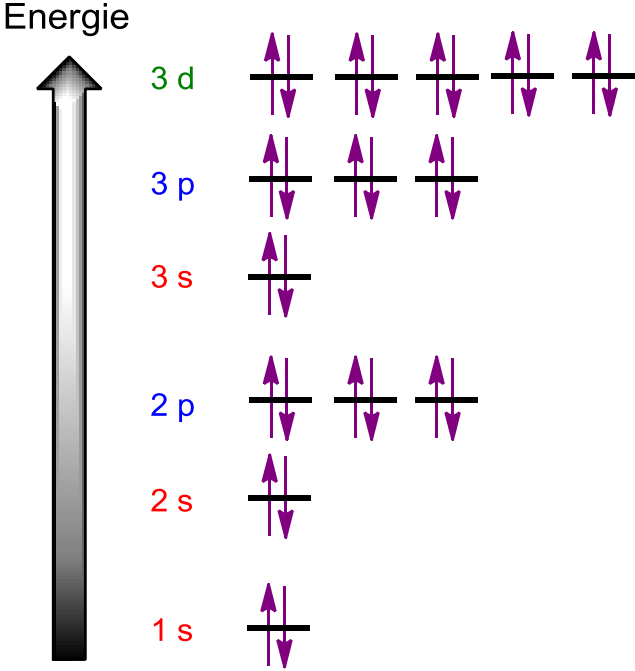
orbital s



orbital p

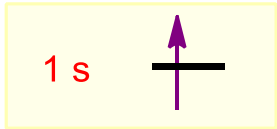


orbital d



# Elektronové konfigurace vybraných prvků

Vodík  ${}^1\text{H}$

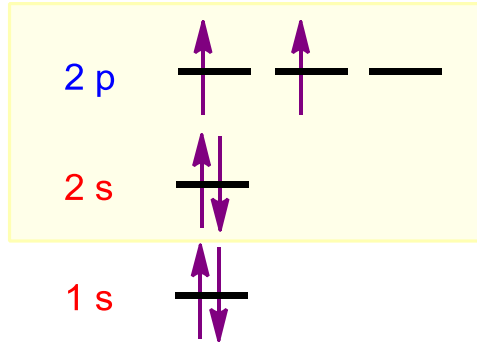


1 elektron

$1s^1$

1 valenční elektron

Uhlík  ${}^{12}\text{C}$

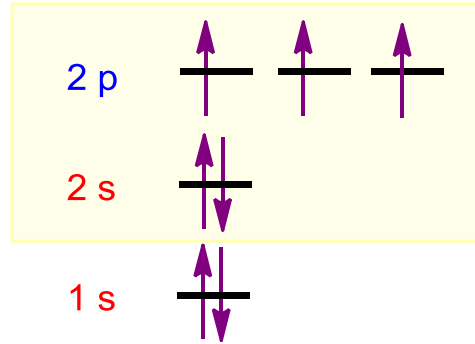


6 elektronů

$1s^2 2s^2 2p_x^1 2p_y^1$

4 valenční elektrony

Dusík  ${}^{14}\text{N}$

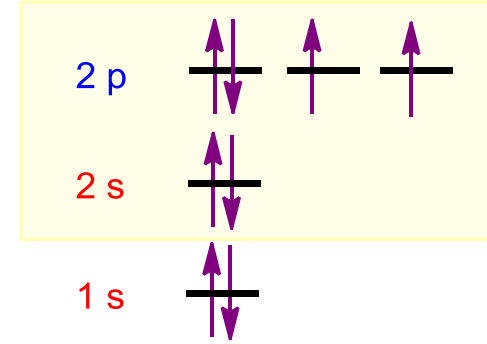


7 elektronů

$1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1$

5 valenčních elektronů

Kyslík  ${}^{16}\text{O}$



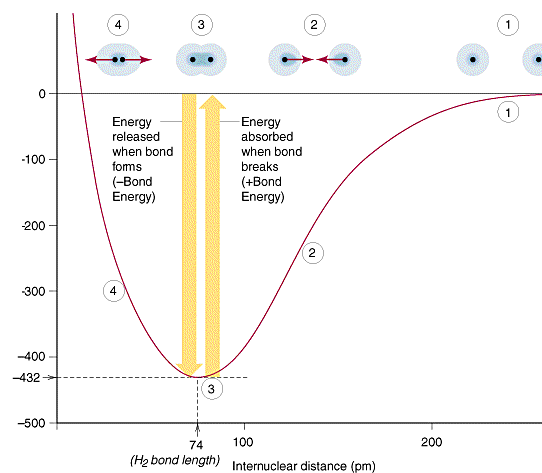
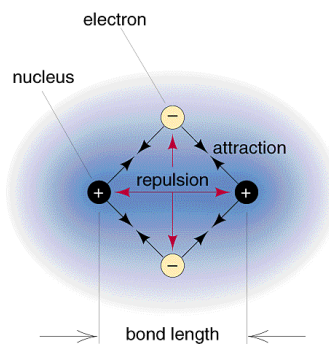
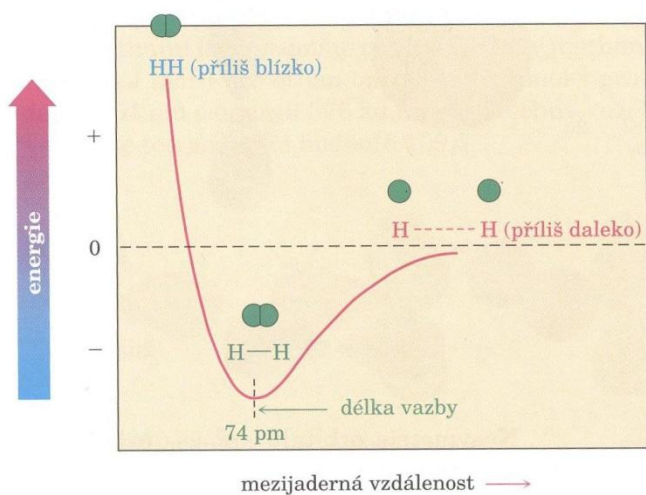
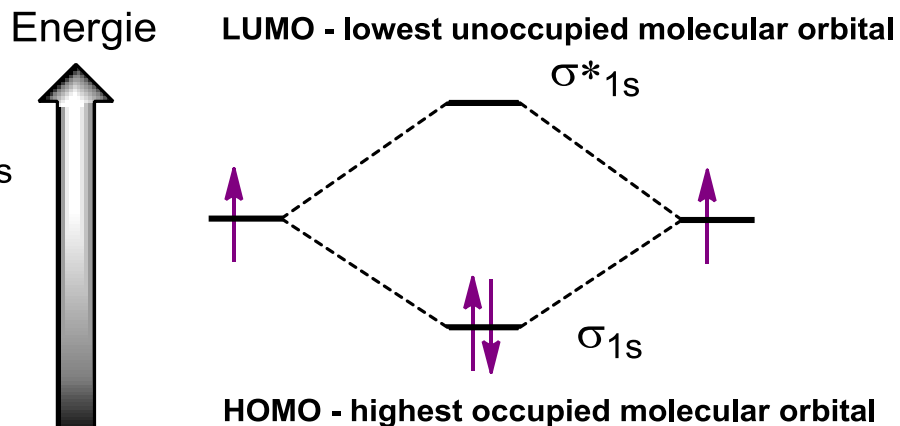
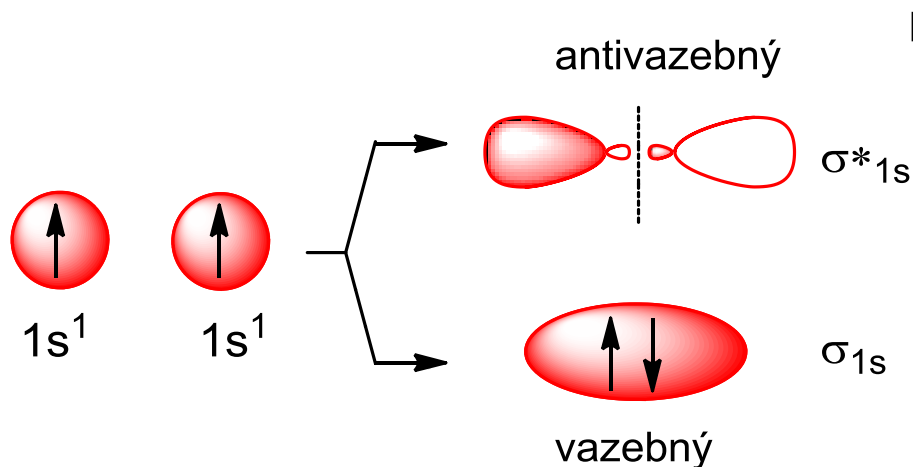
8 elektronů

$1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$

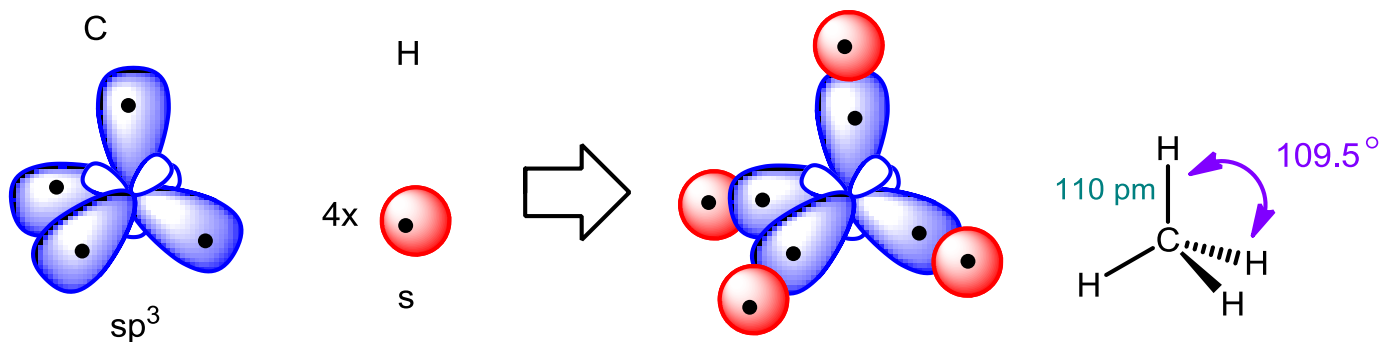
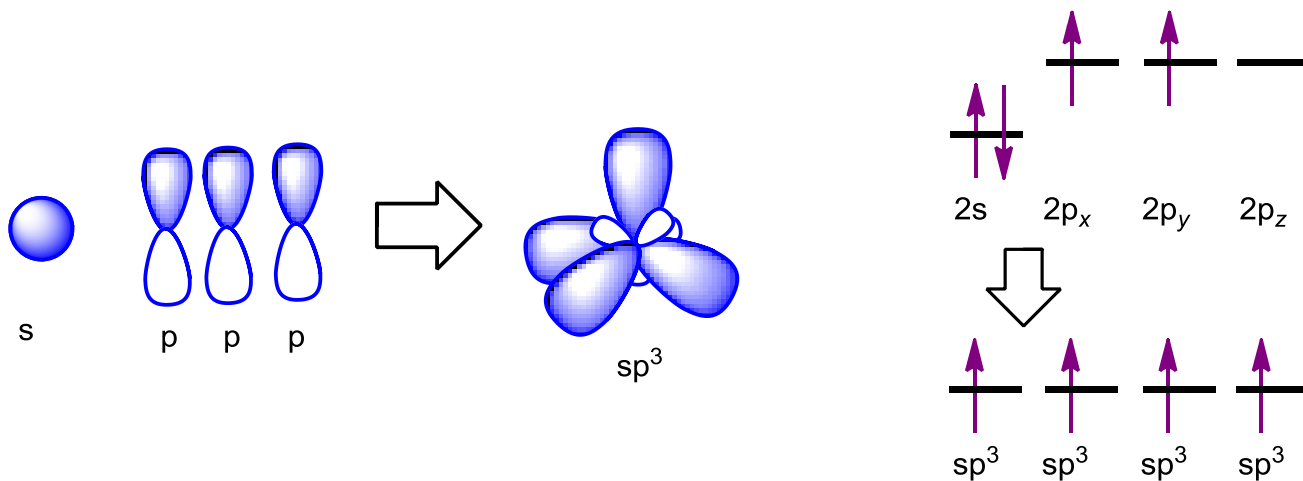
6 valenčních elektronů

# Molekulové orbitály - molekula H<sub>2</sub>

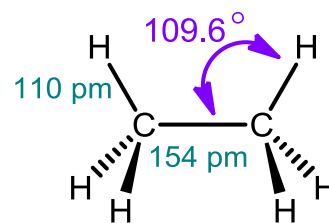
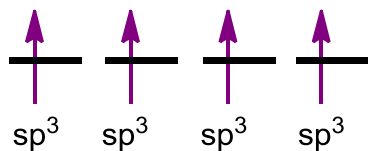
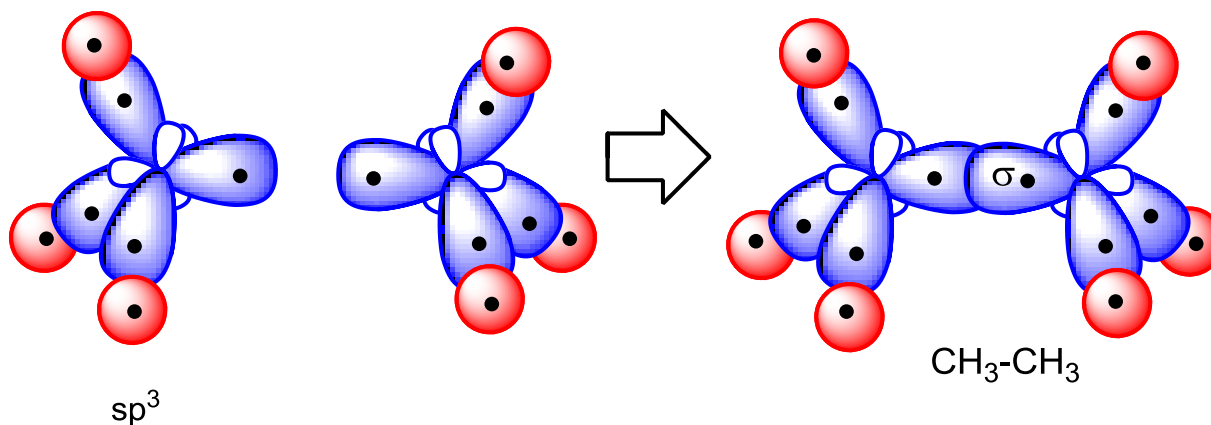
atomové orbitály      molekulové orbitály



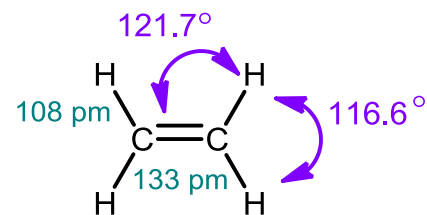
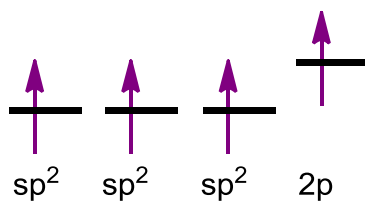
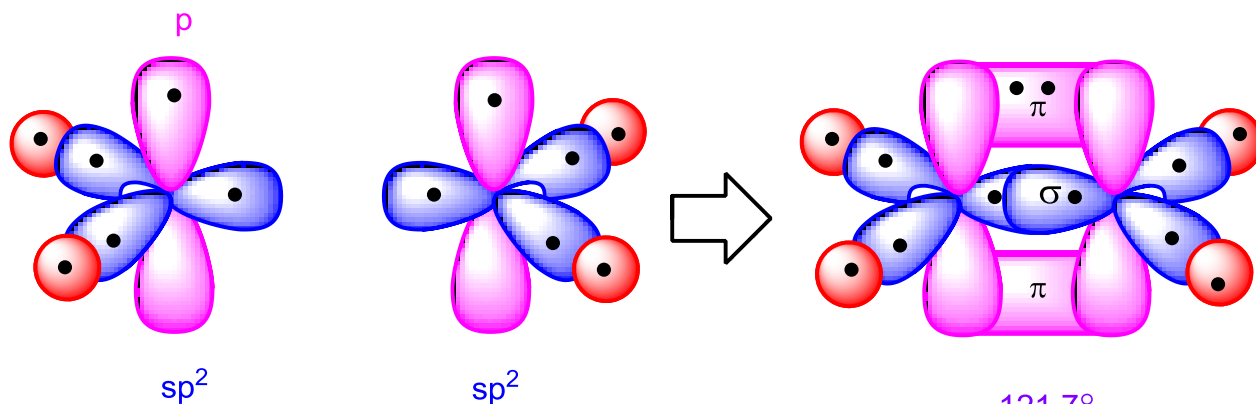
# Molekulové orbitály – hybridizace C



# Molekulové orbitály – jednoduchá vazba C-C, molekula ethanu

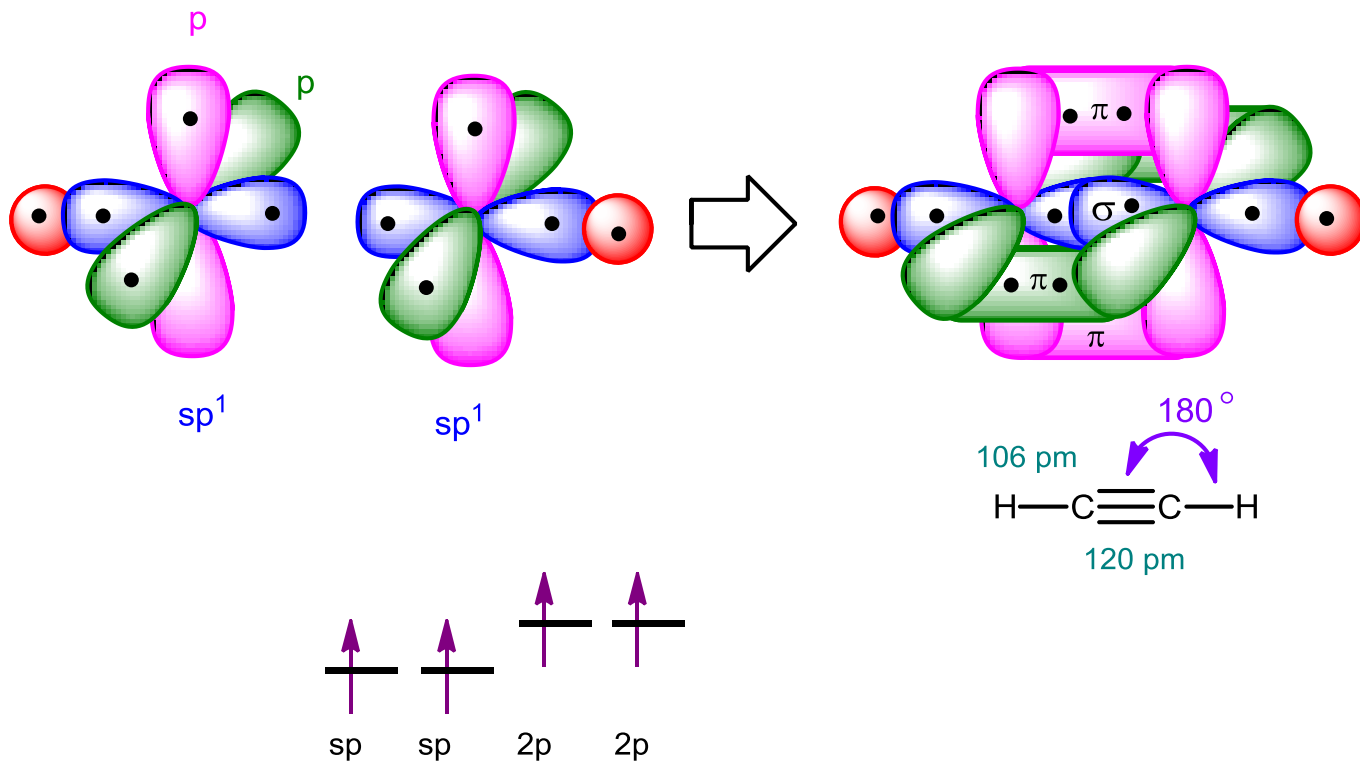


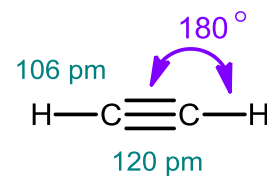
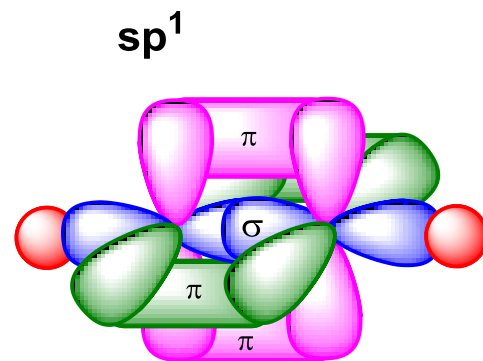
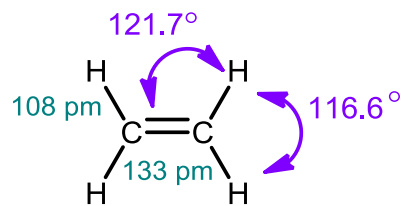
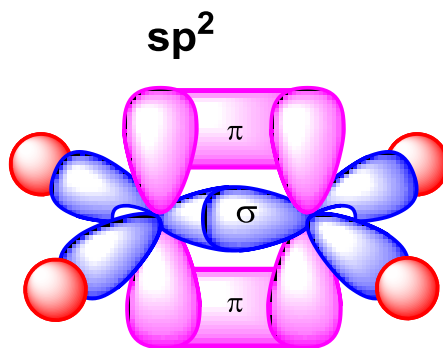
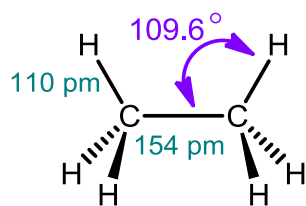
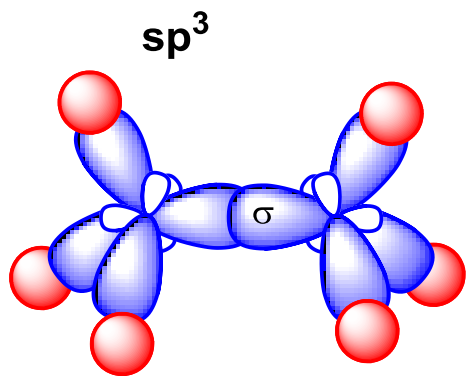
# Molekulové orbitály – dvojná vazba C=C, molekula ethenu



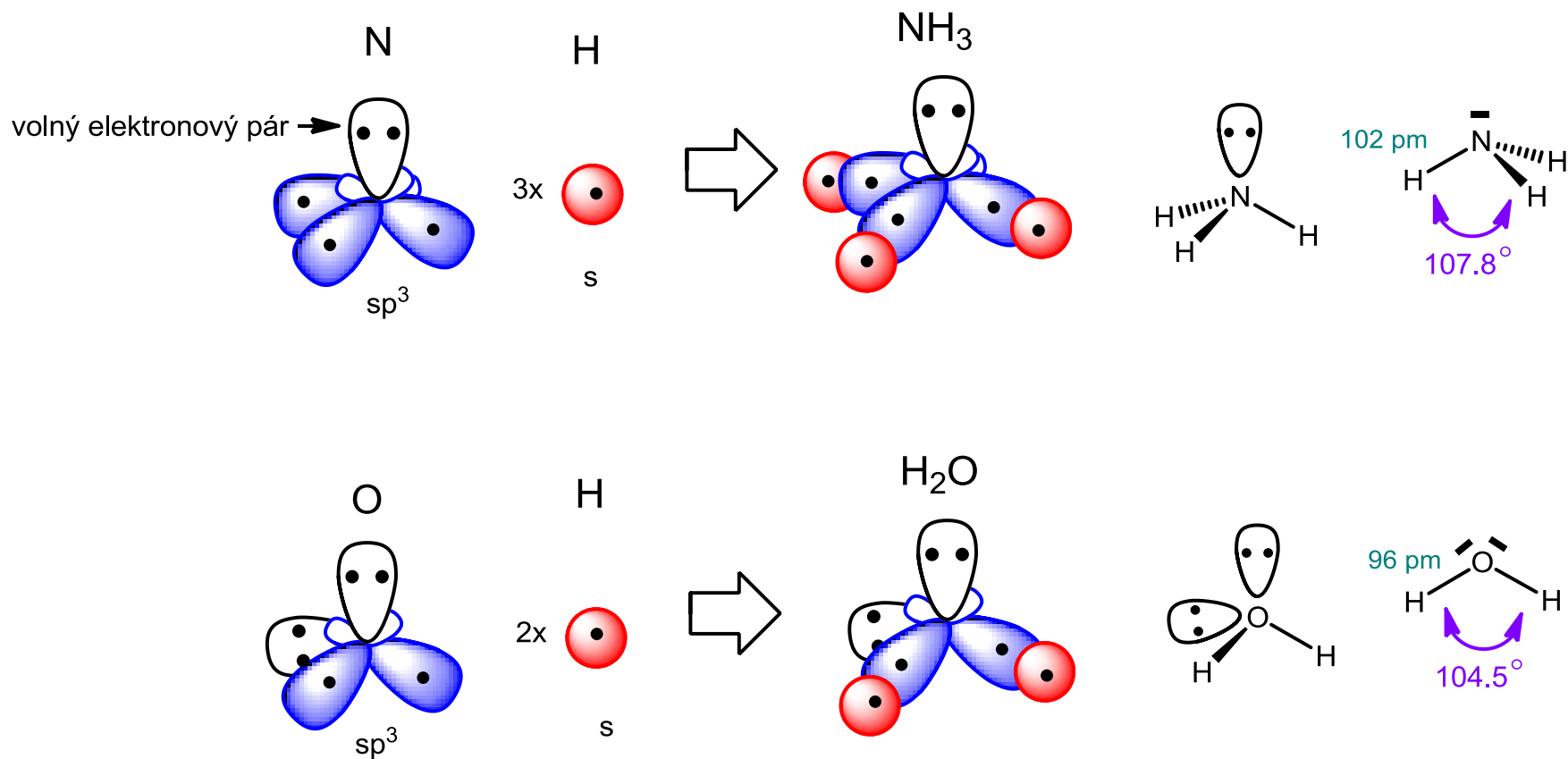


# Molekulové orbitály – trojná vazba $C\equiv C$ , molekula ethynu





# Molekulové orbitály – hybridizace N a O



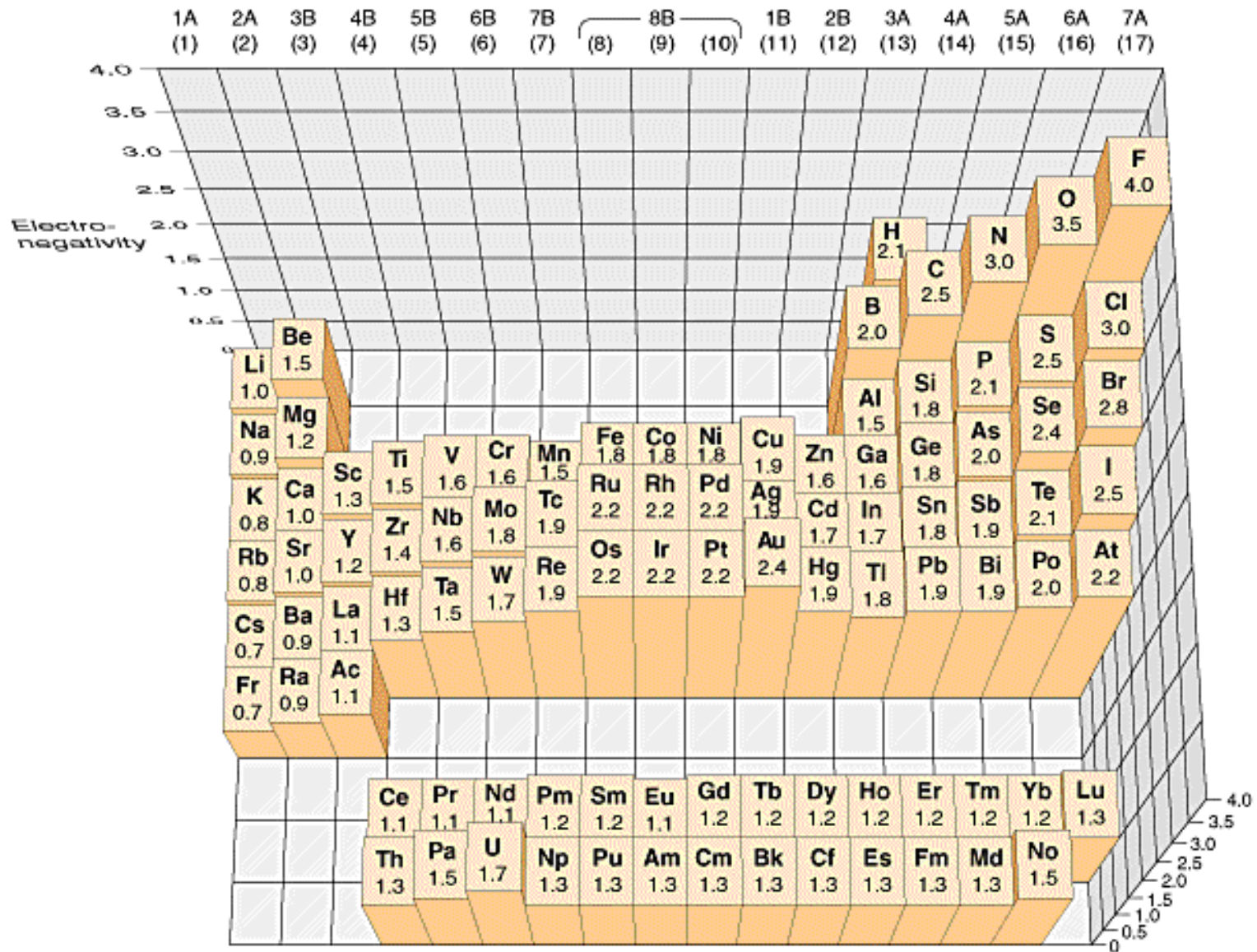
Tabulka 1.2. Elektronové konfigurace prvních 18 prvků.

Atomové číslo	Prvek	Počet elektronu v každém orbitalu					Konfigurace
		1s	2s	2p	3s	3p	
1	H	1					$1s^1$
2	He	2					$1s^2$
3	Li	2	1				$1s^2 2s^1$
4	Be	2	2				$1s^2 2s^2$
5	B	2	2	1			$1s^2 2s^2 2p^1$
6	C	2	2	2			$1s^2 2s^2 2p^2$
7	N	2	2	3			$1s^2 2s^2 2p^3$
8	O	2	2	4			$1s^2 2s^2 2p^4$
9	F	2	2	5			$1s^2 2s^2 2p^5$
10	Ne	2	2	6			$1s^2 2s^2 2p^6$
11	Na	2	2	6	1		$1s^2 2s^2 2p^6 3s^1$
12	Mg	2	2	6	2		$1s^2 2s^2 2p^6 3s^2$
13	Al	2	2	6	2	1	$1s^2 2s^2 2p^6 3s^2 3p^1$
14	Si	2	2	6	2	2	$1s^2 2s^2 2p^6 3s^2 3p^2$
15	P	2	2	6	2	3	$1s^2 2s^2 2p^6 3s^2 3p^3$
16	S	2	2	6	2	4	$1s^2 2s^2 2p^6 3s^2 3p^4$
17	Cl	2	2	6	2	5	$1s^2 2s^2 2p^6 3s^2 3p^5$
18	Ar	2	2	6	2	6	$1s^2 2s^2 2p^6 3s^2 3p^6$

Tabulka 1.3. Valenční elektrony prvních 18 prvků

Skupina							
I	II	III	IV	V	VI	VII	VIII
H·							He:
Li·	Be· ·	B· ·	C· ·	N· ·	O· ·	F· ·	Ne: ·
Na·	Mg· ·	Al· ·	Si· ·	P· ·	S· ·	Cl· ·	Ar: ·

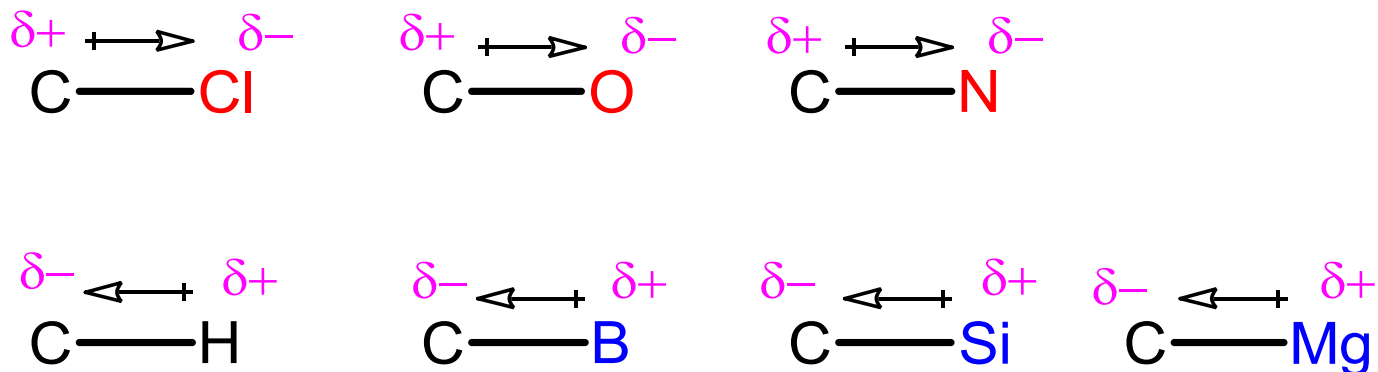
# Elektronegativita prvků



# Polarita vazby, induktivní efekt

U kovalentní vazby mezi rozdílnými atomy, nebude elektronový pár oběma atomy sdílen stejně. Jeden atom bude přitahovat elektrony více a jeden méně, dojde k tvorbě tzv. **parciálního náboje** na jednotlivých atomech.

Vzniká **polární kovalentní vazba**.

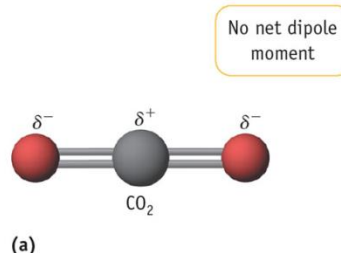


Posun valenčních elektronů označujeme u polárních kovalentních vazeb jako **induktivní efekt**.

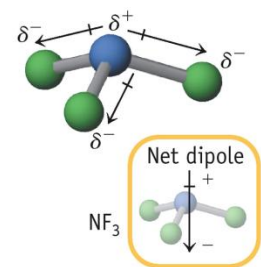
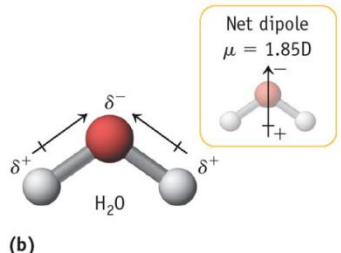
Atomy nebo funkční skupiny, které přitahují elektrony silněji než vodík vykazují **-I efekt**.

Atomy nebo funkční skupiny, které přitahují elektrony slaběji než vodík vykazují **+I efekt**.

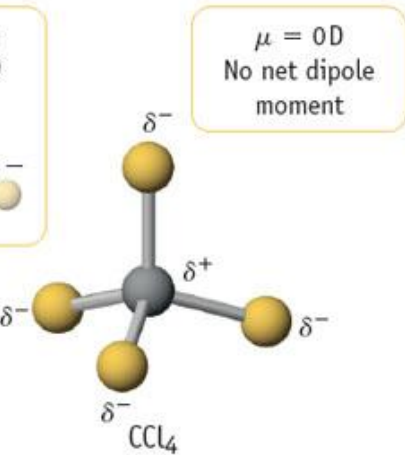
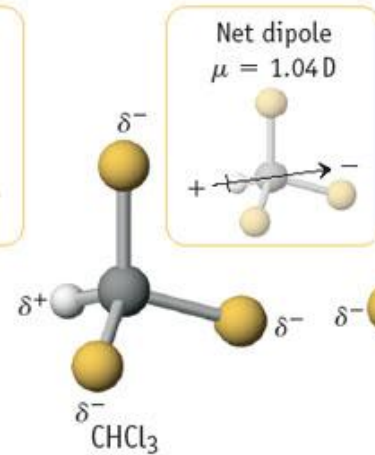
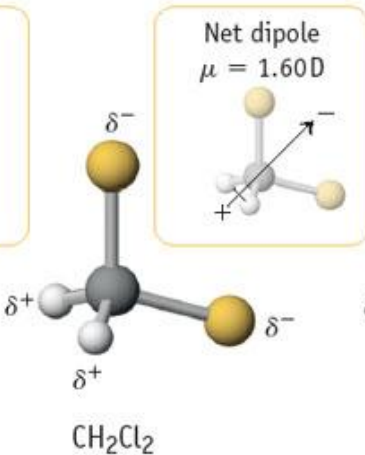
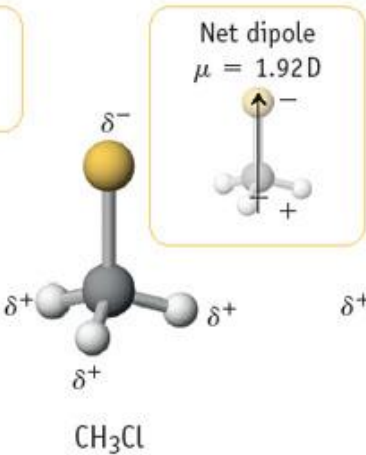
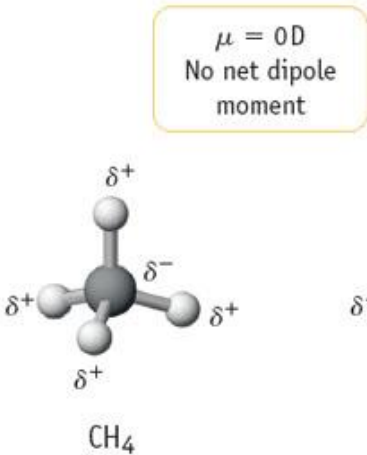
# Dipólový moment



© 2006 Brooks/Cole - Thomson



© 2006 Brooks/Cole - Thomson



© 2006 Brooks/Cole - Thomson



# Disociační energie vazeb

## Average Bond Enthalpies (kJ/mol)

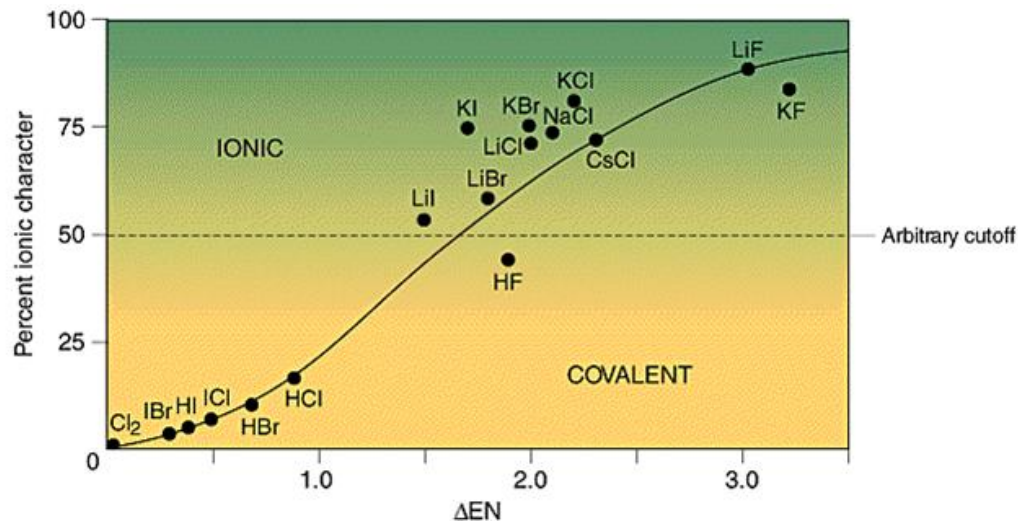
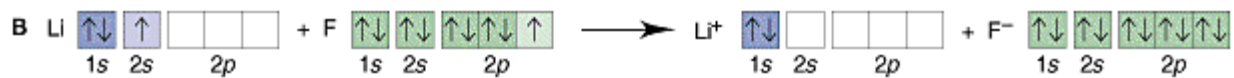
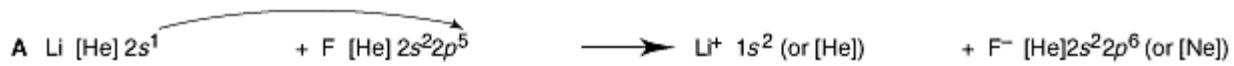
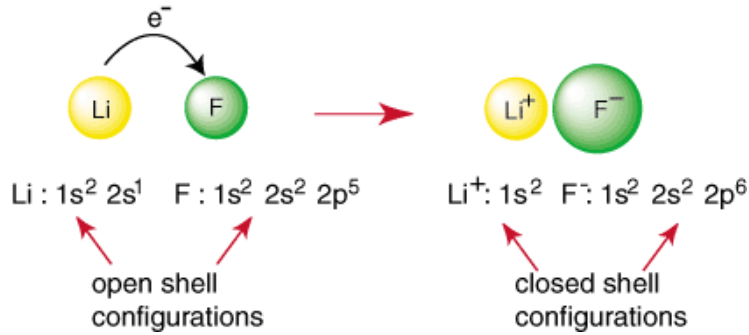
### Single Bonds

C—H	413	N—H	391	O—H	463	F—F	155
C—C	348	N—N	163	O—O	146	Cl—F	253
C—N	293	N—O	201	O—F	190	Cl—Cl	242
C—O	358	N—F	272	O—Cl	203	Br—F	237
C—F	485	N—Cl	200	O—I	234	Br—Cl	218
C—Cl	328	N—Br	243	S—H	339	Br—Br	193
C—Br	276	H—H	436	S—F	327	I—Cl	208
C—I	240	H—F	567	S—Cl	253	I—Br	175
C—S	259	H—Cl	431	S—Br	218	I—I	151
Si—H	323	H—Br	366	S—S	266		
Si—Si	226	H—I	299				
Si—C	301						
Si—O	368						

### Multiple Bonds

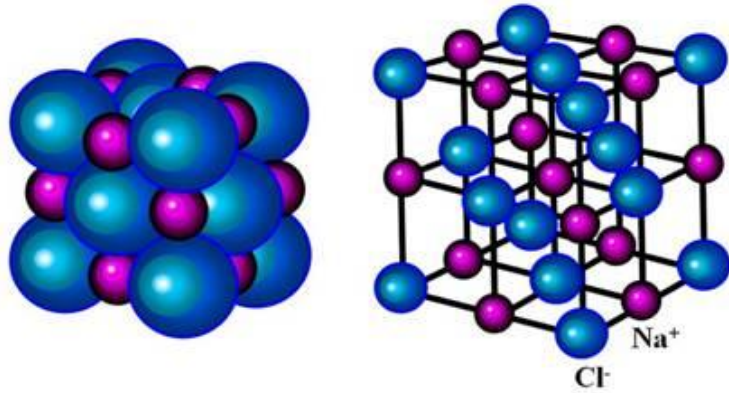
C=C	614	N=N	418	O <sub>2</sub>	495
C≡C	839	N≡N	941	S=O	523
C=N	615			S=S	418
C≡N	891				
C=O	799				
C≡O	1072				

# Iontová vazba

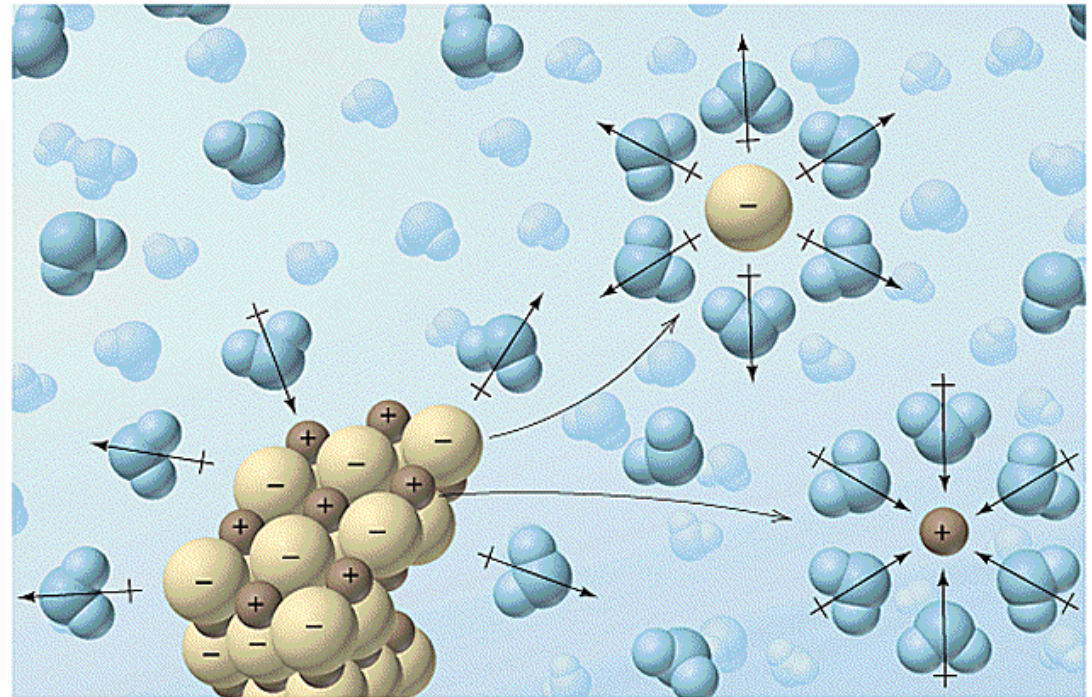
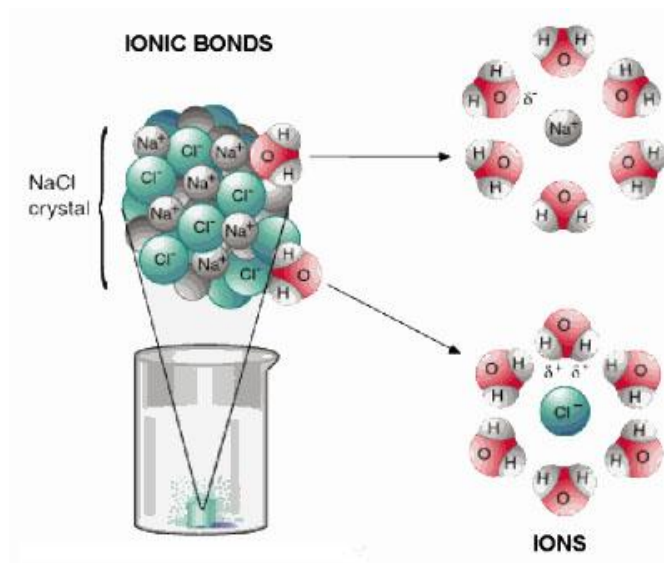


# Struktura iontových sloučenin (solí)

## Pevné skupenství – krystalová mřížka

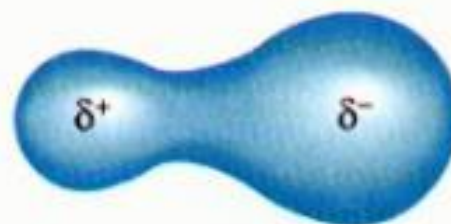


## Vodný roztok – solvatace iontů

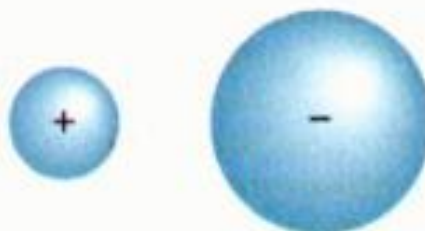




Nonpolar covalent bond

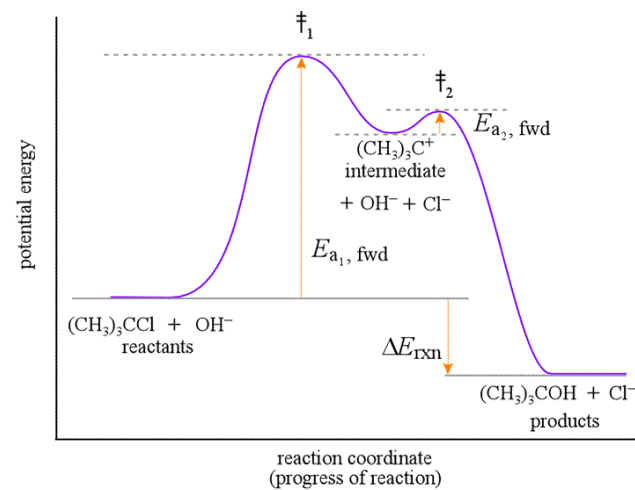
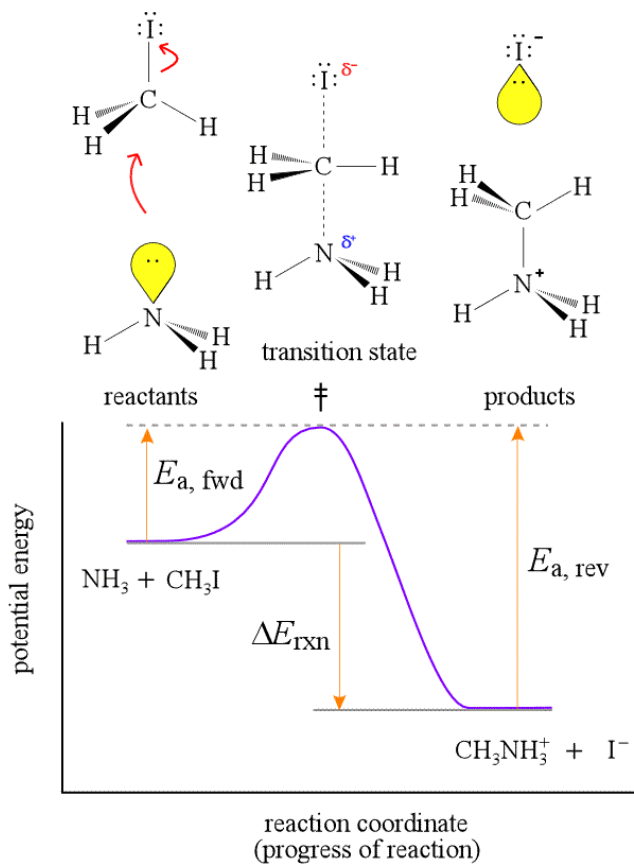
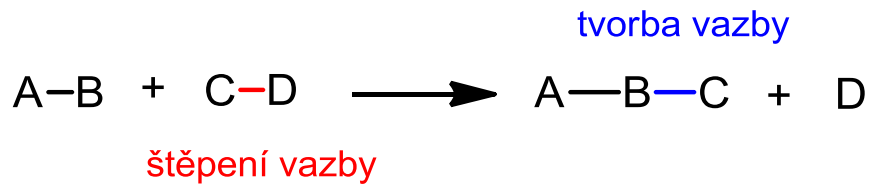
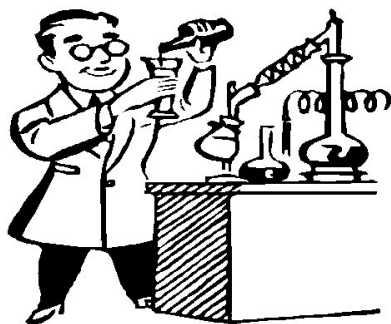


Polar covalent bond

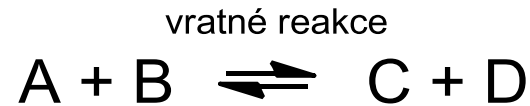


Ionic bond

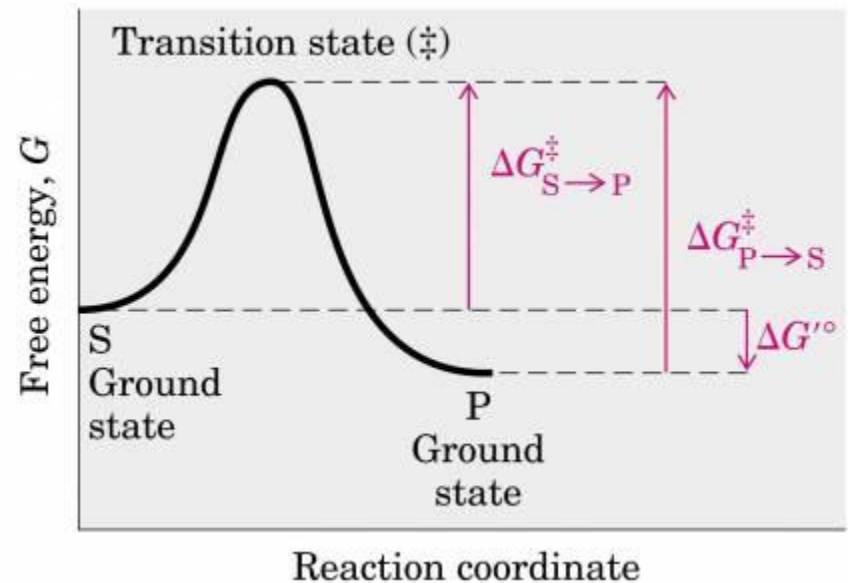
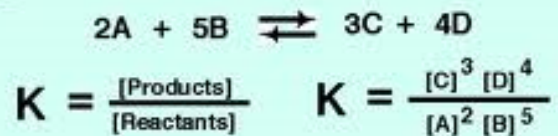
# Chemická reakce – štěpení a tvorba vazeb



# Vratné reakce a reakční termodynamika



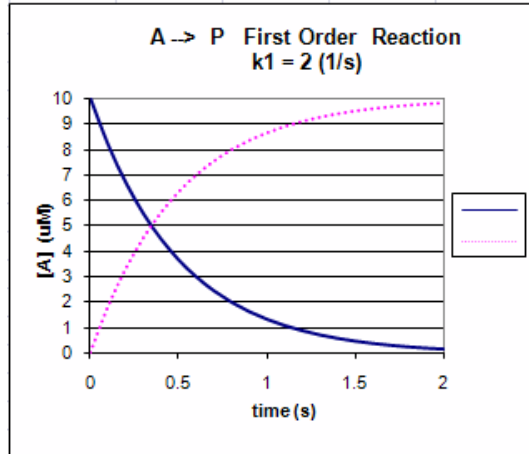
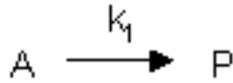
## Rovnovážná konstanta



Exotermní reakce –  $\Delta G < 0$

Endotermní reakce –  $\Delta G > 0$

# Reakční kinetika

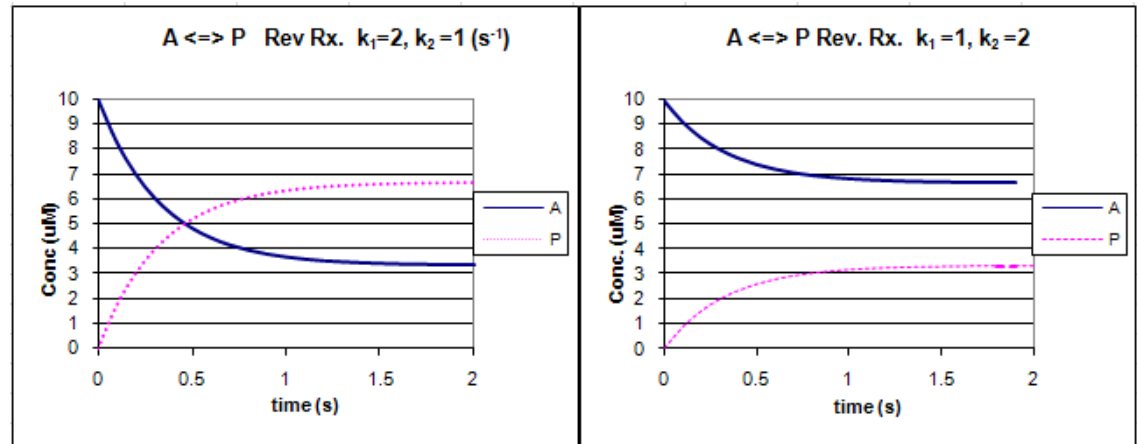
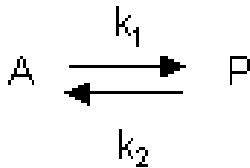


Eyringova rovnice

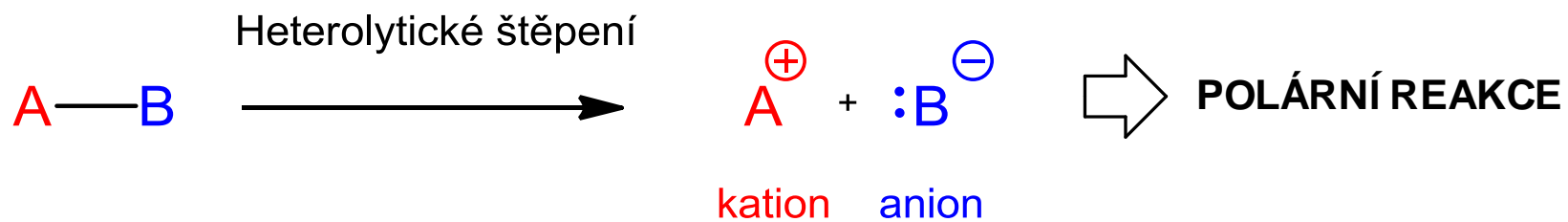
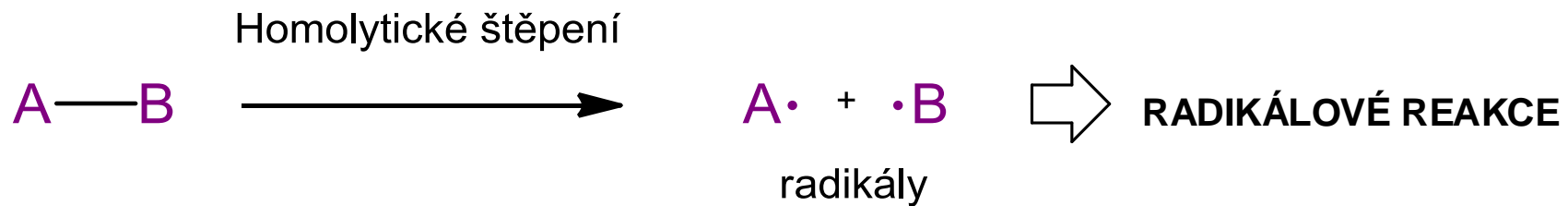
$$k = \frac{k_B T}{h} e^{-\frac{\Delta G^\ddagger}{RT}}$$

se zvyšující se teplotou reakční rychlost roste

Vratná reakce



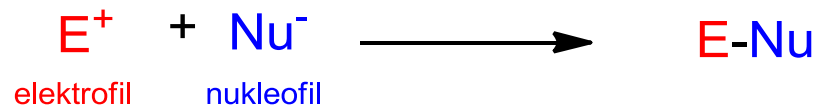
# Štěpení vazeb





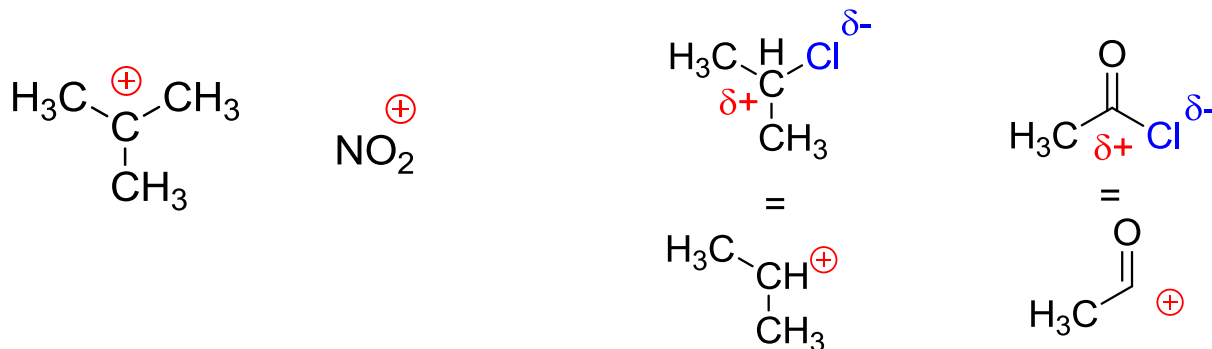
# Elektrofilní a nukleofilní reagenty

## Polární reakce



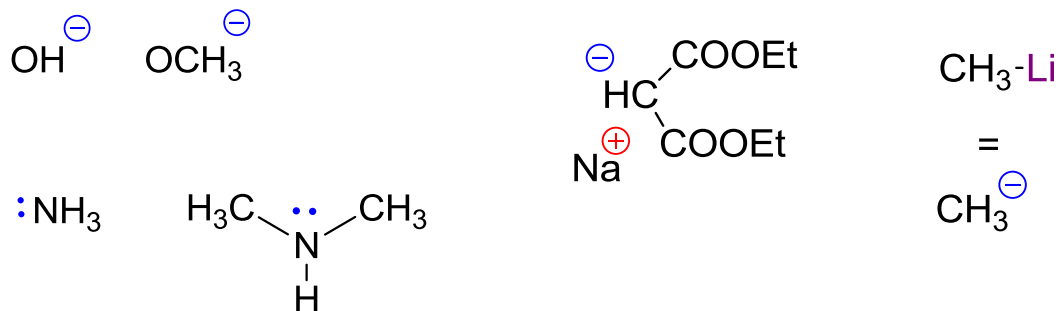
### Elektrofilní reagent:

- má afinitu k záporně nabitým částicím
- Jde o kation nebo elektronově chudou neutrální molekulu



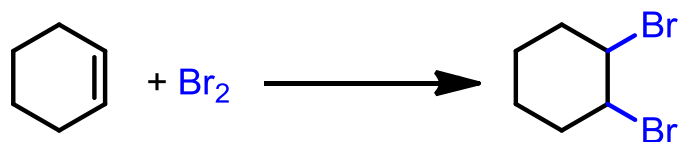
### Nukleofilní reagent:

- má afinitu ke kladně nabitým částicím
- Jde o anion nebo elektronově bohatou neutrální molekulu

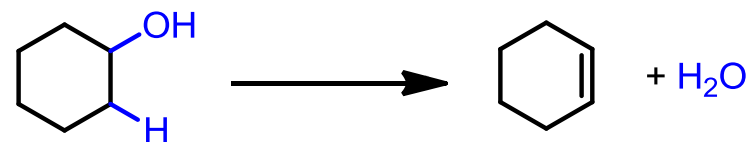
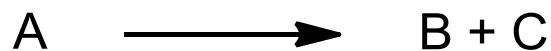


# Typy reakcí v organické chemii

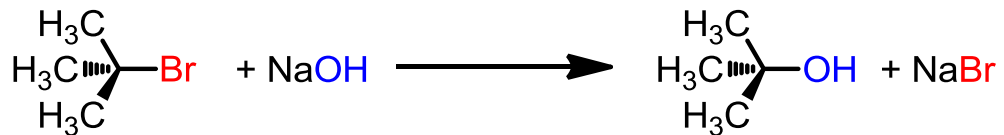
## ADICE



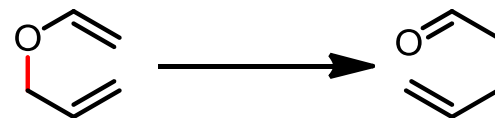
## ELIMINACE



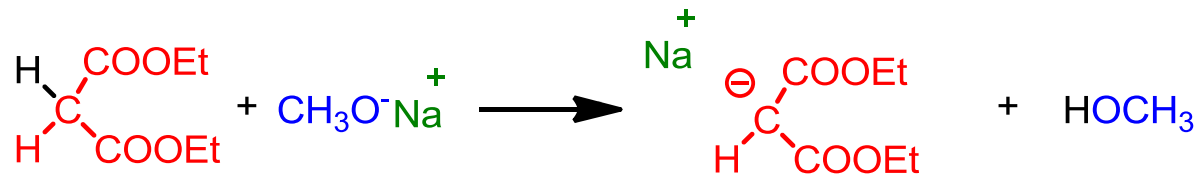
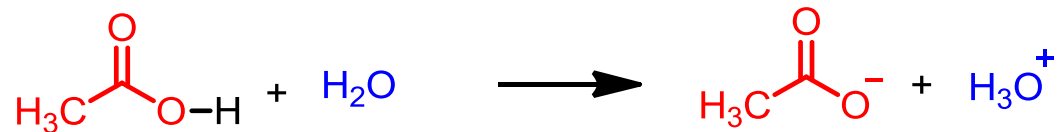
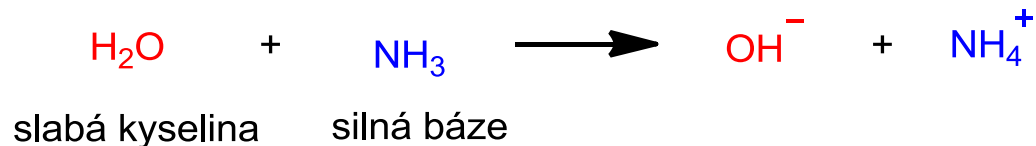
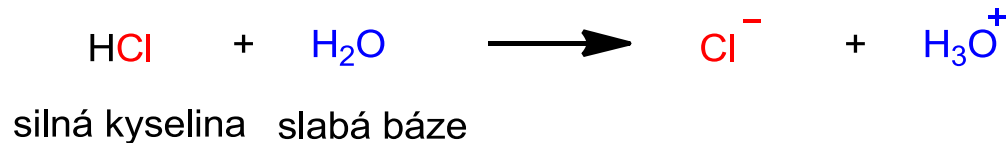
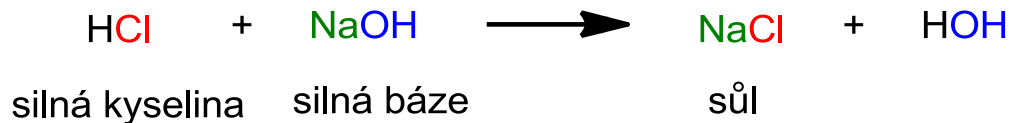
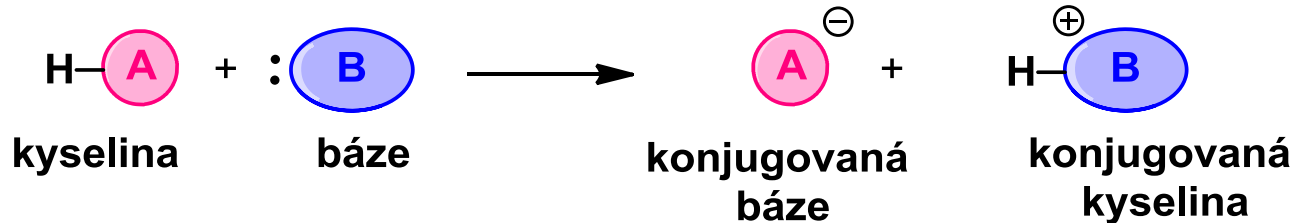
## SUBSTITUCE



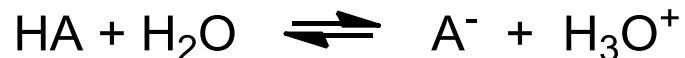
## PŘESMYKY



# Kyseliny a báze - Brønstedovy



# Kyseliny a báze - Brønstedovy


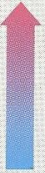


Rovnovážná konstanta  $K = \frac{[\text{H}_3\text{O}^+][\text{A}^-]}{[\text{HA}][\text{H}_2\text{O}]}$

Konstanta kyselosti  $K_a = K[\text{H}_2\text{O}] = \frac{[\text{H}_3\text{O}^+][\text{A}^-]}{[\text{HA}]}$

Síla kyseliny se uvádá v  $\text{p}K_a = -\log K_a$

**TABULKA 2.3** Relativní síla některých běžných kyselin a jejich konjugovaných bází

	Kyselina	Název	$\text{p}K_a$	Konjugovaná báze	Název	
slabší kyselina 	$\text{CH}_3\text{CH}_2\text{OH}$	ethanol	16,00	$\text{CH}_3\text{CH}_2\text{O}^-$	ethoxidový ion	silnější báze 
	$\text{H}_2\text{O}$	voda	15,74	$\text{HO}^-$	hydroxidový ion	
	$\text{HCN}$	kyanovodíková kyselina	9,31	$\text{CN}^-$	kyanidový ion	
	$\text{CH}_3\text{COOH}$	octová kyselina	4,76	$\text{CH}_3\text{COO}^-$	acetátový ion	
	$\text{HF}$	kyselina fluorovodíková	3,45	$\text{F}^-$	fluoridový ionn	
	$\text{HNO}_3$	kyselina dusičná	-1,3	$\text{NO}_3^-$	dusičnanový ion	
silnější kyselina	$\text{HCl}$	kyselina chlorovodíková	-7,0	$\text{Cl}^-$	chloridový ion	slabší báze

# Kyseliny a báze - Lewisovy

obsazený orbital



Lewisova báze

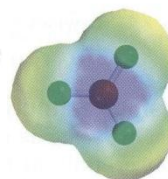
+

neobsazený orbital

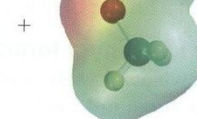


Lewisova kyselina

→

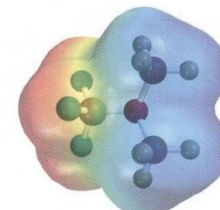


fluorid boritý

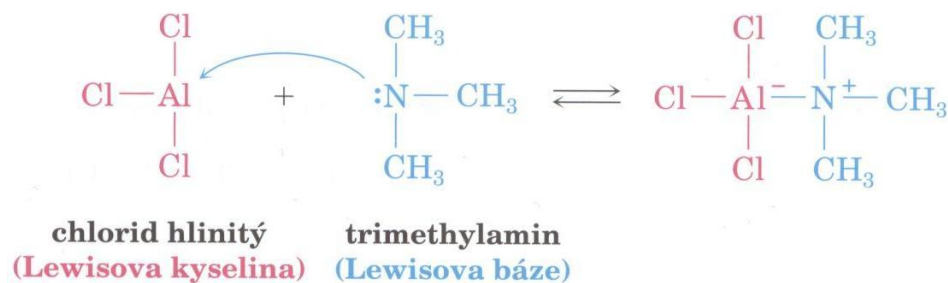
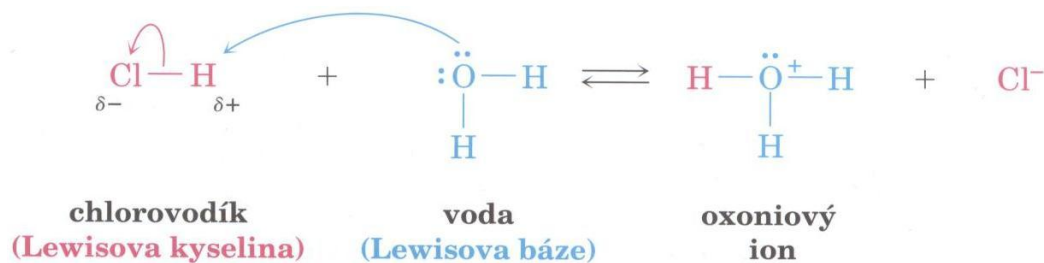


dimethylether

⇌

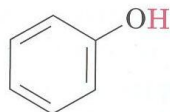
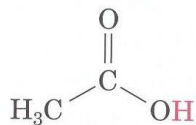


Lewisův acidobazický komplex



**některé Lewisovy kyseliny**

neutrální donory protonů:



karboxylová kyselina

fenol

alkohol

**některé Lewisovy báze**

některé kationty:



některé sloučeniny kovů



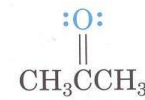
alkohol



ether



aldehyd



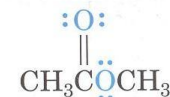
keton



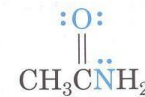
acylchlorid



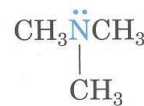
karboxylová kyselina



ester



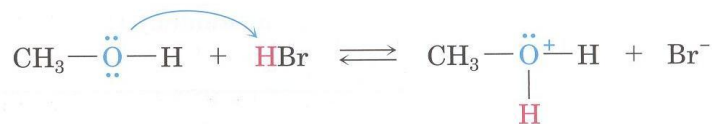
amid



amin



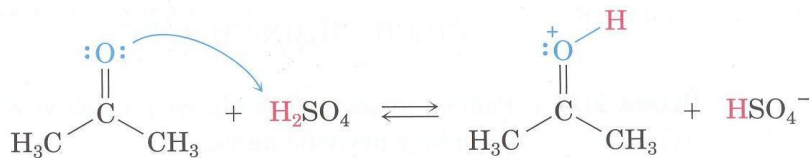
sulfid



methanol  
(báze)

bromovodík  
(kyselina)

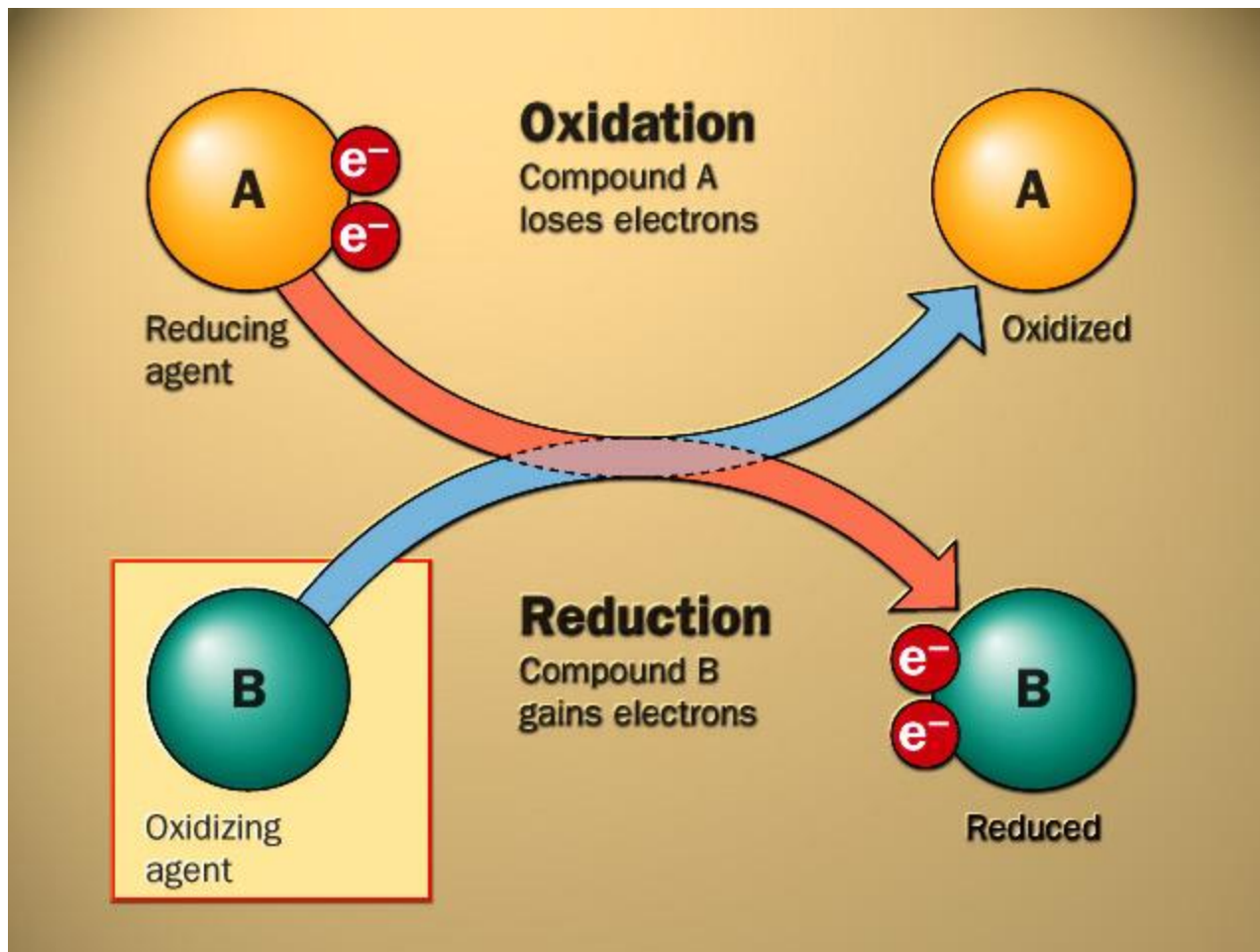
methyloxonium-bromid



aceton  
(báze)

kyselina sírová

# Redoxní reakce – oxidace a redukce



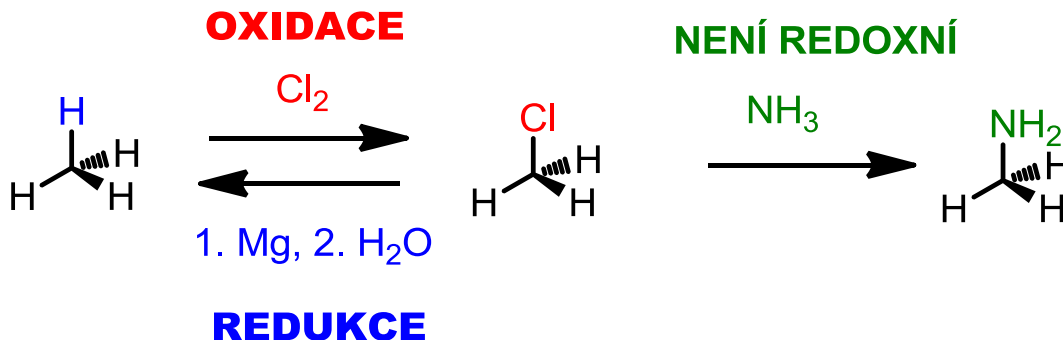
# Redoxní reakce – oxidace a redukce

**Oxidace** – dochází ke **snížení elektronové hustoty na atomu uhlíku**

- tvorbou vazeb C-O, C-N, C-X nebo C=C
- zánikem vazeb C-H

**Redukce** – dochází ke **zvýšení elektronové hustoty na atomu uhlíku**

- zánikem vazeb C-O, C-N, C-X nebo C=C
- tvorbou vazeb C-H nebo C-kov

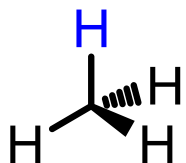




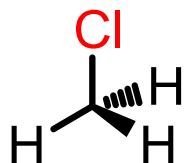
# Redoxní reakce – oxidační stupeň

## Deriváty methanu

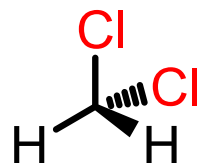
-IV



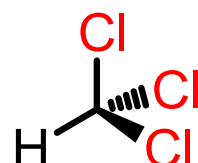
-II



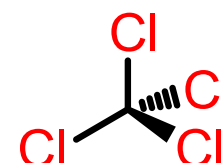
0



+II



+IV



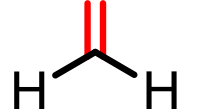
MgBr



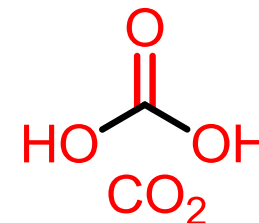
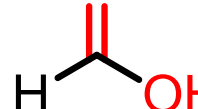
OH



O



O



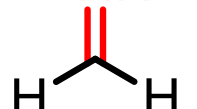
Li



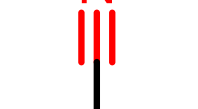
NH<sub>2</sub>



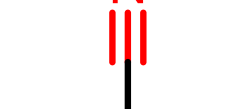
NH



N



N



Br

# Redoxní reakce – oxidace a redukce

Deriváty vyšších uhlovodíků (R = alkyl)

